

Phase diagram in 2D Fröhlich model of metal at arbitrary carrier density: pseudogap *versus* doping

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Abstract

It is shown that in 2D system of the fermions with simplest indirect boson-induced attraction (through the Einstein phonon exchange as an example) along with the normal and superconducting phases there arises a new (called "abnormal normal" or pseudogap) one where the absolute value of the order parameter is finite but its phase is a random quantity. It is important that this new phase really exists at low carriers density only, i.e. it shrinks when doping increases. The relevance of the results obtained with dependence of pseudogap on doping in high-temperature superconductors is speculated.

Key words: 2D metal, arbitrary carrier density, normal phase, abnormal normal phase, pseudogap, superconducting phase, Berezinskii-Kosterlitz-Thouless phase

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1 Introduction

An adequate description of the physical properties of high-temperature superconductors (HTSCs) is one of the most important problems of the modern solid state physics (see, for example, review [1]). And among the most debatable questions on HTSCs is the question about the so called pseudogap (or spin gap) which is experimentally observed in normal state samples with lowered carrier density n_f . The matter is that HTSCs represent systems with relatively easy changeable value of n_f what is interesting and important both from experimental and from theoretical points of view. In particular, the underdoped samples reveal a lot of strange anomalies concerning their spectral, magnetic, thermodynamic and other observables (among them there is the pseudogap which has been seen in ARPES experiments [2, 3, 4] and now widely discussed [5, 6, 7]). Moreover, even the definition itself "underdoped" ("overdoped") HTSC sample is related to the presence (absence) of such anomalies.

On the other hand, the possibility of changing n_f value is crucial for the theory and puts the general problem of the crossover from composite boson superfluidity (underdoped regime, or small n_f) to Cooper pairing when n_f increases (overdoped regime). This crossover was already studied for the systems of different dimensionalities: 3D [8] and quasi-2D [9]. As for 2D case, it has been considered for temperature $T = 0$ only [8, 10] what is conditioned by the Hohenberg-Mermin-Wagner theorem which forbids any long-range order in such systems at finite T because of long-wave fluctuations of the charged order parameter.

Formation of inhomogeneous condensate, or the Berezinskii-Kosterlitz-Thouless (BKT) phase, is possible, but its consistent study is connected with some difficulties. Nevertheless, this case was already explored in 2+1 relativistic field model [11] where, as it is known, concentration effects are not justifiable. They are known for some nonrelativistic models (see, for example, [12]), but the BKT equation in this paper was obtained without taking into account the existence of neutral order parameter ρ ($\neq 0$). Its introduction and use, as it was shown in [13], is very important and leads to formation of a new phase with $\rho \neq 0$ which separates normal phase and another one, which is also normal, since superconducting

properties are absent there as well.

Below an attempt is made to study the above mentioned crossover and the new phase formation possibility. In contrast to [13], where this question was studied for a 2D four-fermion (4F) model, we shall consider a more realistic Fröhlich model. It will be shown that the unknown phase in this case not just exists, but appears mainly at low carrier density what is essentially different from the 4F-case. Such a result promises that the models with an indirect attractive fermion-fermion interaction may be suitable to account for the unusual features in the normal phase behaviour of HTSCs.

2 Model and main equations

Let us choose the Fröhlich model Hamiltonian density in the standard form:

$$H(x) = -\psi_\sigma^\dagger(x) \left(\frac{\nabla^2}{2m} - \mu \right) \psi_\sigma(x) + g\varphi(x)\psi_\sigma^\dagger(x)\psi_\sigma(x) + H_{ph}(\varphi(x)), (x = \mathbf{r}, t), \quad (1)$$

where $\psi_\sigma(x)$ is a fermion field; m and $\sigma = \uparrow, \downarrow$ are an effective mass and a spin of the fermions, μ is their chemical potential which fixes n_f ; $\varphi(x)$ is a phonon field operator and g is a fermion-phonon coupling constant. We use Pauli matrices $I, \tau_x, \tau_y, \tau_z$ and put $\hbar = k_B = 1$.

In (1) H_{ph} is the Hamiltonian of free phonons, which results in the simplest expression for the phonon propagator (in the Matsubara temperature formalism)[14]

$$D(i\Omega_n) = -\frac{\omega_0^2}{\Omega_n^2 + \omega_0^2}, \quad \Omega_n = 2n\pi T \quad (2)$$

with ω_0 as Einstein phonon frequency and n as an integer. In principle, (2) corresponds to a propagator of any massive bosonic excitations by which fermions can exchange¹.

With the purpose to calculate the phase diagram it is necessary to find the thermodynamic potential of the system. In the case of the 4F model it can be obtained by making use of

¹In spite of its simplicity such a model is rather close to HTSCs with their developed quadrupolar mode spectra - optical phonons and dd -excitons [1]. Exchange of these excitations leads to short-range interaction between fermions. It, however, does not include spin excitations (almost massless in HTSCs) which can provide the long-range inter-carrier interaction what, of course, needs a separate study.

the well-developed Hubbard-Stratonovich method in which the statistical sum Z can be represented by a path integral over the fermionic $\psi_\sigma(x)$ and the complex Hubbard-Stratonovich $\phi(x) = V \langle \psi_\uparrow^\dagger \psi_\downarrow^\dagger \rangle$ fields (V is the 4F-interaction constant).

As it was shown earlier [15, 13], in 2D case it is convenient to pass from ϕ and ϕ^* fields to new variables, namely: the absolute value ρ and the phase θ , where $\phi(x) = \rho(x) \exp[-2i\theta(x)]$, and to perform simultaneously the spinor transformation

$$\psi_\sigma(x) = \chi_\sigma(x) \exp[i\theta(x)], \quad (3)$$

where $\chi_\sigma(x)$ corresponds to a neutral fermi-particle field. Such a substitution allows to represent Z in the following form

$$Z = \int \rho \mathcal{D}\rho \mathcal{D}\theta \exp \left[-\beta \int \Omega(\rho(x), \theta(x)) dx \right], \quad (\beta = 1/T) \quad (4)$$

where Ω is the effective quantum thermodynamic potential in terms of $\rho(x)$ and $\theta(x)$ variables. This representation proves to be very useful and leads to (at $\rho(x) = \text{const}$ and expansion in $\nabla\theta(x)$ up to $(\nabla\theta(x))^2$) the effective Hamiltonian which is similar to that of the XY-model. As a result, the equation for T_{BKT} in the latter model can be directly used for the case under consideration. The solution of whole the set of the self-consistent equations for ρ , μ and T_{BKT} was given in [13].

This approach is however inapplicable in the more complex case of indirect interaction model for which the local Hubbard-Stratonovich fields can not be introduced. At the same time, by making use of the Cornwall-Jackiw-Tomboulis formalism [16] it is possible to obtain classical thermodynamic potential which depends on bilocal $\langle \psi_\downarrow(x) \psi_\uparrow(y) \rangle$ and $\langle \psi_\uparrow^\dagger(x) \psi_\downarrow^\dagger(y) \rangle$ fields (or, more exactly, on the full fermion Green function (see below)) though, strictly speaking, this potential does not satisfy Eq. (4) exactly. The corresponding effective action (equivalent to Ω in (4)) in two-loop approximation can be calculated and (in the Nambu representation [17]) takes the form

$$\beta\Omega[\mathcal{G}] = -\text{Tr} \left(\text{Ln} \mathcal{G}^{-1} \mathcal{G}_0 + \mathcal{G} \mathcal{G}_0^{-1} - 1 \right) + \frac{g^2}{2} \text{Tr} \mathcal{G} \tau_z D \tau_z \mathcal{G}, \quad (5)$$

where Tr includes integration over 2D space \mathbf{r} and imaginary time $0 \leq \tau \leq \beta$ as well as the

standard trace operation;

$$\begin{aligned}\mathcal{G}^{-1} &= -I\partial_\tau + \tau_z \left(\frac{\nabla^2}{2m} + \mu \right) + \tau_+ \phi^* + \tau_- \phi; \\ \mathcal{G}_0^{-1} &= \mathcal{G}^{-1}(\rho = 0)\end{aligned}\tag{6}$$

are the full and free fermion Green functions, and D was defined in (2). We also use the normalization condition $\mathcal{G}_0 = \mathcal{G}_0(\mu = 0)$ under the symbol Ln in (5).

The stationary condition $\delta\Omega(\mathcal{G})/\delta\mathcal{G} = 0$ results in the well-known Schwinger-Dyson equation² for the inverse full fermion Green function

$$\mathcal{G}^{-1} = \mathcal{G}_0^{-1} - g^2 \tau_z \mathcal{G} \tau_z D.\tag{7}$$

Substituting (7) into (5) one can obtain a simpler expression for $\Omega(\mathcal{G})$ where the phonon Green function (2) is already omitted

$$\beta\Omega(\mathcal{G}) = -\text{Tr} \left[\text{Ln} \mathcal{G}^{-1} \mathcal{G}_0 + \frac{1}{2} (\mathcal{G} \mathcal{G}_0^{-1} - 1) \right].\tag{8}$$

To find the potential Ω as a function of phase gradient $\nabla\theta(x)$ and absolute value ρ it is necessary to make the transformation (3). Then one obtains for (6):

$$\begin{aligned}\mathcal{G}^{-1} &= -I\partial_\tau + \tau_z \left(\frac{\nabla^2}{2m} + \mu \right) + \tau_x \rho - \\ &\quad \tau_z \left(\partial_\tau \theta + \frac{\nabla \theta^2}{2m} \right) + iI \left(\frac{\nabla^2 \theta}{2m} + \frac{\nabla \theta \nabla}{m} \right) \equiv G^{-1}(\rho) - \Sigma(\partial\theta); \\ \mathcal{G}_0^{-1} &\equiv G_0^{-1} - \Sigma(\partial\theta).\end{aligned}\tag{9}$$

Since the low energy dynamics is mainly determined by the phase fluctuations and corresponds to the region where spatially homogeneous order parameter $\rho \neq 0$ it is sufficient to be restricted the expansion in terms of Ω in $\nabla\theta(x)$ only; for instance, the Green function (9) $\mathcal{G} = G + G \Sigma_{n=0}^\infty (G \Sigma)^n$. Then the desirable effective potential (8) can be divided it two parts: $\Omega = \Omega_{pot}(\rho) + \Omega_{kin}(\rho, \nabla\theta)$, where in $(\nabla\theta)^2$ approximation

$$\begin{aligned}\beta\Omega_{kin}(\rho, \nabla\theta) &= \text{Tr} \left[G \Sigma + \frac{1}{2} G \Sigma G \Sigma - G_0 \Sigma - \frac{1}{2} G_0 \Sigma G_0 \Sigma + \right. \\ &\quad \left. \frac{\rho}{2} \tau_x G (G \Sigma + G \Sigma G \Sigma) \right].\end{aligned}\tag{10}$$

²In fact it coincides with the Eliashberg equation [17] when the renormalization factor is $Z(i\omega_n) = 1$.

Assuming then that $\rho(i\omega_n) = \text{const}$ one obtains from (10) after somewhat tedious but otherwise straightforward calculation

$$\Omega_{kin} = \frac{T}{2} \int_0^\beta d\tau \int d^2\mathbf{r} J(\mu, T, \rho(\mu, T)) (\nabla\theta)^2, \quad (11)$$

where

$$J(\mu, T, \rho(\mu, T)) = \frac{1}{2\pi} (\sqrt{\mu^2 + \rho^2} + \mu + 2T \ln \left[1 + \exp \left(-\frac{\sqrt{\mu^2 + \rho^2}}{T} \right) \right] - \frac{T}{\pi} \left[1 - \frac{\rho^2}{4T^2} \frac{\partial}{\partial(\rho^2/4T^2)} \right] \int_{-\mu/2T}^\infty dx \frac{x + (\mu/2T)}{\cosh^2 \sqrt{x^2 + \rho^2/4T^2}}. \quad (12)$$

Note that in comparison with the 4F model [13] the last expression contains one more term with the derivative.

The equation for the temperature T_{BKT} of the BKT transition can be written after direct comparison of Ω_{kin} (11) with the Hamiltonian of the XY-model which has the same form [18]; hence

$$\frac{\pi}{2} J(\mu, T_{BKT}, \rho(\mu, T_{BKT})) = T_{BKT}. \quad (13)$$

To complete a set of selfconsistent equations which allow us to trace the dependence of T_{BKT} on n_f the equations for ρ and μ have also to be given.

In particular the equation for $\rho(i\omega_n)$ is nothing else but (7) with $\nabla\theta = 0$, i.e. the Green function G of the neutral fermions replaces \mathcal{G} , so that (7) in frequency-momentum representation takes the form

$$\rho(i\omega_n) = g^2 T \sum_{m=-\infty}^\infty \int \frac{d^2\mathbf{k}}{(2\pi)^2} \frac{\rho(i\omega_m)}{\omega_m^2 + \varepsilon^2(\mathbf{k}) + \rho^2(i\omega_m)} \frac{\omega_0^2}{(\omega_m - \omega_n)^2 + \omega_0^2}, \quad (14)$$

where $\omega_n = (2n+1)\pi T$ is the Matsubara fermionic frequency [17].

Analytical study of this equation as well as obtaining both (12) and the number equation is possible only if one supposes that $\rho(i\omega_n) = \text{const}$ ³.

Finally, the number equation which follows from the condition $v^{-1} \partial \Omega[\mathcal{G}] / \partial \mu = -n_f$ (where v is a volume of the system) and is crucial for crossover description has to be added to (13) and (14) for self-consistency; so one comes to

$$\sqrt{\mu^2 + \rho^2} + \mu + 2T \ln \left[1 + \exp \left(-\frac{\sqrt{\mu^2 + \rho^2}}{T} \right) \right] = 2\epsilon_F, \quad (15)$$

³For the case $T = 0$ this assumption was checked in [19].

where $\epsilon_F = \pi n_f / m$ is the Fermi energy of 2D fermions with the simplest quadratic dispersion law. Thus, in the case under consideration all unknown quantities (ρ, μ and T_{BKT}) are functions of n_f .

3 Analysis of the solutions

It is natural to guess that in contrast to the accepted XY-model in the superconducting model there exists one more critical temperature, also dependent on n_f , where the complete order parameter vanishes. This critical temperature, T_ρ , can be found from (14) and (15) by putting $\rho = 0$ (what in accordance with these equations derivation corresponds to the mean-field approximation). As a result, with temperature decreasing 2D metal passes from normal phase ($T > T_\rho$) to another one where averaged homogeneous (charged) order parameter $\langle \phi(x) \rangle = 0$, or, what is the same, superconductivity is absent, but chargeless order parameter $\rho \neq 0$. It is very important that the pseudogap is formed just in the temperature region $T_{BKT} < T < T_\rho$, because, as it follows from above formulas (see, for instance, (14), (15)), ρ , which depends on n_f and T , enters all spectral characteristics of 2D metal in the same way as the superconducting gap $\Delta(T)$ enters into corresponding expressions for ordinary superconductors. It explains why this, new phase can be called the "abnormal normal" phase or, better, pseudogap one. The density of states near ϵ_F in the pseudogap is definitely less than in the normal phase, but is not equal zero as in superconducting one.

The phase diagram of the system is presented in fig.1. Both curves for T_ρ and T_{BKT} as functions of n_f can be obtained by numerical calculation. As for their asymptotic behaviour can be established analytically.

Indeed, it is not difficult to be convinced that the asymptotics for $T_\rho(n_f)$ and $T_{BKT}(n_f)$ have the forms:

a) when ratio $\epsilon_F / \omega_0 \ll 1$ (very low fermion density, or local pair case) the first of them satisfies the equation $T_\rho \ln(T_\rho / \epsilon_F) = \omega_0 \exp(-2/\lambda)$ which immediately results in $\partial T_\rho(n_f) / \partial n_f|_{n_f \rightarrow 0} \rightarrow \infty$. At the same time the temperature T_{BKT} here has another carrier density depen-

dence: $T_{BKT} = \epsilon_F/2$ what in its turn means that it is equal to the number of composite bosons. It means that in this density region $T_\rho/T_{BKT} \gg 1$.

b) in the case $\epsilon_F/\omega_0 \gg 1$ (very large fermion density, or Cooper pair case) one comes to standard BCS value: $T_\rho = (2\gamma\omega_0/\pi) \exp(-1/\lambda) \equiv T_{BCS}^{MF} = (2\gamma/\pi)\Delta_{BCS}$ (Δ_{BCS} is the one-particle BCS gap at $T = 0$). In other words, the temperature T_ρ becomes equal to its BCS value⁴. The T_{BKT} asymptotics in this case is not so evident and requires more detailed consideration.

Firstly, it is naturally to suppose that for large n_f values $T_{BKT} \rightarrow T_\rho$. Then it is necessary to check the dependence of ρ on T as $T \rightarrow T_\rho$. For that the equation (14) can be transformed to:

$$\frac{1}{\lambda} = \int_0^\infty dx \left(\frac{\tanh \sqrt{x^2 + \rho^2/4T^2}}{\sqrt{x^2 + \rho^2/4T^2}} - \frac{\tanh \sqrt{x^2 + \rho^2/4T^2} - \tanh(\omega_0/2T)}{2(\sqrt{x^2 + \rho^2/4T^2} - \omega_0/2T)} - \frac{\tanh \sqrt{x^2 + \rho^2/4T^2} + \tanh(\omega_0/2T)}{2(\sqrt{x^2 + \rho^2/4T^2} + \omega_0/2T)} \right) \quad (16)$$

(where it was used that in this concentration region the ratio $\mu/2T_\rho \simeq \epsilon_F/2T_\rho \gg 1$).

Because usually $\omega_0/2T_\rho \gg 1$, only very small x give the main contribution to the integral (16) (it is seen from the limit $\rho/2T_\rho \rightarrow 0$ when $\epsilon_F/\omega_0 \rightarrow \infty$). Therefore the latter expression takes the approximate form:

$$\frac{1}{\lambda} = \int_0^\infty dx \left(\frac{\tanh \sqrt{x^2 + \rho^2/4T^2}}{\sqrt{x^2 + \rho^2/4T^2}} - \frac{1}{x + \omega_0/2T} \right). \quad (17)$$

On the other hand, the condition $\rho = 0$ in (17) leads to the equation

$$\frac{1}{\lambda} = \int_0^\infty dx \left(\frac{\tanh x}{x} - \frac{1}{x + \omega_0/2T_\rho} \right). \quad (18)$$

for T_ρ . From (17) and (18) it directly follows that

$$\int_0^\infty dx \left(\frac{\tanh x}{x} - \frac{\tanh \sqrt{x^2 + \rho^2/4T^2}}{\sqrt{x^2 + \rho^2/4T^2}} \right) = \ln \frac{T_\rho}{T}.$$

⁴Being equal (in mean field approximation only) these temperatures (T_ρ and T_{BCS}^{MF}) are in fact different: if T_{BCS}^{MF} immediately falls down to zero as fluctuations are taken into account, T_ρ does not and is renormalized only.

Then using the approximation

$$\frac{\tanh \sqrt{x^2 + \rho^2/4T^2}}{\sqrt{x^2 + \rho^2/4T^2}} \simeq \begin{cases} 1 - 3^{-1} [x^2 + \rho^2/4T^2], & x \leq 1 \\ x^{-1} - \rho^2/8T^2 x^3, & x > 1 \end{cases}$$

one easily comes to expression needed:

$$\rho \simeq 2.62T_\rho \sqrt{T_\rho/T - 1}. \quad (19)$$

Remind that the generally accepted 3D result is $\Delta_{BCS}(T) = 3.06T_{BCS}^{MF} \sqrt{T_{BCS}^{MF}/T - 1}$ [14] and this small difference can be explained by the above approximation what, however, is suitable for the following below qualitative discussion (see next Section).

The last dependence has to be substituted in equation (13). And because of $\mu/2T_{BKT} \simeq \epsilon_F/2T_{BKT} \gg 1$, and $\rho(T_{BKT})/2T_{BKT} \ll 1$ when $T_{BKT} \rightarrow T_\rho$ this equation can be written as

$$\frac{\epsilon_F}{4T_{BKT}} \left[1 - \frac{\rho^2}{4T_{BKT}^2} \frac{\partial}{\partial(\rho^2/4T_{BKT}^2)} \right] \int_0^\infty dx \left(\frac{1}{\cosh^2 x} - \frac{1}{\cosh^2 \sqrt{x^2 + \rho^2/4T_{BKT}^2}} \right) = 1. \quad (20)$$

At last, using expansion in $\rho/2T_{BKT}$ in integral (20), the latter can be transformed to

$$\frac{a\epsilon_F}{8T_{BKT}} \left(\frac{\rho}{2T_{BKT}} \right)^4 = 1, \quad (21)$$

where the numerical constant

$$a = \int_0^\infty dx \frac{\tanh^2 x - x^{-1} \tanh x + 1}{2x^2 \cosh x} \simeq 1.98.$$

Combining now (19) and (21) one comes to the final relation between T_ρ and T_{BKT} for large carrier density:

$$T_{BKT} \simeq T_\rho (1 - 1.17 \sqrt{T_\rho/\epsilon_F}), \quad (22)$$

i.e. T_{BKT} as a function of n_f approaches T_ρ (or T_{BCS}^{MF}).

4 Discussion

Thus, in the considered model of 2D metal with indirect interection of carriers, along with the normal phase ($\rho = 0$), there exist pseudogap and superconducting (here - BKT) phases which

in fact correspond to the cases of absent, uncorrelated and correlated pairs, respectively. Despite the simplicity of the model and assumptions made above, the strong dependence of the critical temperatures T_{BKT} and T_ρ on carrier density is evidently shown. Pseudogap phase really exists when $\epsilon_F \leq 100T_{BCS}^{MF}$ (or $(T_\rho - T_{BKT})/T_\rho \geq 0.1$ (see (22))). This conclusion agrees qualitatively with the existence of unusual spectral peculiarities in some underdoped HTSCs (for example, YBCO [2, 3, 4]). There are many speculations about the nature of this pseudogap phase (in particular, the spin-gap conception (see [20]) is also very popular). Our results give hopes that "the low-density phenomena" in HTSCs can be (at least, principally) explained in the framework of a rather standard boson-exchange approach though the simplest phonon model considered can hardly be available for description of real HTSC compounds.

It must be also noted that unlike this model the 4F one predicts the pseudogap phase existence at any fermion densities [13]. It means that in the case 2D boson-exchange model with, as shown above, "saturated" critical temperatures as functions of doping, the definitions of "underdoped" and "overdoped" samples acquire their physical sense. Nevertheless, a point where both $(T_\rho(n_f))$ and $T_{BKT}(n_f)$ curves cross each other is absent. The matter is that the second temperature appears at finite value of ρ only. In this connection it is worth to mention that real HTSCs are not pure 2D, but quasi-2D systems with very weak (mainly, Josephson) tunneling between neighbouring conducting copper-oxide layers. In such a case there can exist one more critical temperature [9]

$$T_c \simeq \frac{T_{BKT}}{\ln(\epsilon_F |\varepsilon_b| / 4t_{||}^2)}, \quad (23)$$

which (at small n_f) defines the formation of usual homogeneous condensate where not only ρ but also the phase θ does not depend on coordinates. In (23) $t_{||}$ is the inter-plane hopping (tunneling) constant, and ε_b is the two-fermion bound state energy [1, 8]. When $T_c < T_{BKT}$ all three temperatures have physical meaning, but when $T_c > T_{BKT}$ (or, as it follows from (23), $t_{||} > 2\Delta_{BCS}$) the BKT phase cannot be formed and pseudogap phase at $T = T_c$ transfers directly to the ordinary superconducting phase.

It cannot be excluded that just such a scenario takes place in HTSC copper oxides. Be-

sides, superconducting phase which appears at $T = T_c$ does not need a finite ρ , so the curves $T_\rho(n_f)$ and $T_c(n_f)$ can in principle cross each other in some point $n_f = n_f^{opt}$ which, thus, separates two different doping regions. One more result following from such a consideration is that the ratio $2\Delta/T_c$ proves to be decreasing function of n_f approaching this ratio canonical BCS value 3.52 at large n_f only what agrees with experimental observation (see [21]).

Although above it was pointed out that the pseudogap phase – BKT phase transition takes place when $\rho \neq 0$ and fluctuations of ρ are not so important as those of θ , it would be interesting to estimate their contributions separately. The one-particle gapless spectrum of the normal phase and especially pseudogap in abnormal normal phase spectrum are also of great interest and need further investigation.

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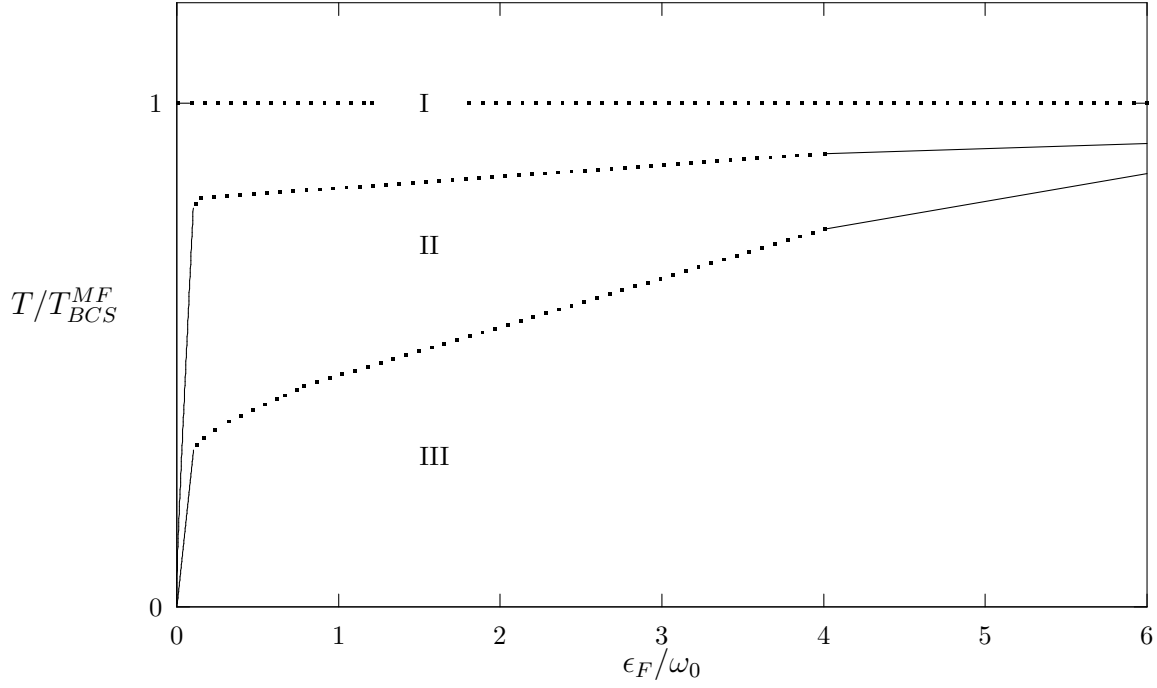


Figure 1: Phase $T - n_f$ diagram of 2D metal with indirect inter-carrier attraction. The solid lines correspond to the calculated (for $\lambda = 0.5$) parts of the functions $T_\rho(n_f)$ and $T_{BKT}(n_f)$, dashed ones guide on the eye. I, II and III show the regions of the normal, abnormal normal and superconducting phases, respectively.